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ESTIMATION OF EXPLOSIVE HAZARD BY COMPUTER[1]

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Abstract. Four parameters from the American Society for Testing and Materials' computer program CHETAH were used to predict energy hazard potential, as defined by consensus grading, into three stability (self-reactivity) categories—nonhazardous chemicals, chemicals capable of hazardous polymerizations or decompositions, and explosives. Out of 34 chemicals for which there was consensus agreement, 31 were correctly assigned to their known classes to yield a total error of 9%—all overestimated. An additional 11 chemicals for which the consensus ratings disagreed were also classified, and appeared to be consistent with one or the other consensus ratings. The addition of two other parameters, heat of polymerization and resonance stabilization of the free radical, reduced the error to one chemical. Classification of over a hundred chemicals, for which the ASTM has compiled experimental shock sensitivity data, falls into 2 categories: nonexplosives and explosives. Using the 4 CHETAH parameters and one structural parameter resulted in total error of about 5%, with the majority of the error being overestimation of hazard potential. It is concluded that the CHETAH program will estimate the self-reactivity hazard of any organic chemical (with 3 or more carbon atoms) with nil underestimation error, and less than 4% overestimation error.

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The American Society for Testing and Materials (ASTM) Committee E-27 on Hazard Potential of Chemicals has been engaged in a broad spectrum of development and standardization of physical and chemical test methods since 1967. In conjunction with the activities of Subcommittee III on Condensed Phase Reactions, the computer program CHETAH (CHEmical Thermodynamics And energy Hazard evaluation) (Seaton *et al* 1974) was developed to be the first of a series of tests to characterize the relative hazard of chemical compounds. This paper describes a significant improvement in the applicability of CHETAH and demonstrates the accuracy of this technique.

Since prediction of hazard potential in advance of manufacture is emphasized, the important case is the one in which no thermodynamic data are available for the chemical in question. CHETAH, therefore, first estimates the thermodynamic properties of the compound. Then it defines the reaction by which the chemical, or mixture of chemicals, can react, in a way consistent with the laws of stoichiometry so as to release the maximum possible amount of energy. It then calculates this maximum heat of the decomposition reaction and 3 other parameters.

CHETAH CRITERIA

1. Maximum enthalpy of decomposition, $\Delta H_{max.}$
2. Heat of combustion-minus heat of decomposition, $\Delta H_{comb.} - \Delta H_{max.}$
3. Oxygen balance.
4. Y, a factor which is equivalent to: $\frac{10 (\Delta H_{max})^2 W}{n}$

where W is the total weight of the reactants in moles and n is the number of atoms of the reactants.

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The program evaluates the potential energy release of the system according to various criteria using empirical correlations with these 4 thermodynamic parameters. CHETAH can also be used to estimate values of the chemical thermodynamic properties, heat capacity, enthalpy, entropy, and heat of combustion, at any temperature between 290° and 1510°K, either for individual compounds or for balanced chemical equations. In the latter case, the program also furnishes the net enthalpy, entropy, and free energy of the reaction.

A number of benefits can be perceived if a computerized approach for hazard evaluation of chemical systems could be demonstrated. Substantial savings in time and cost could be realized in evaluating the hazard potential of new chemiclas—a virtually impossible task if the astronomical number of combinations of nearly 1000 chemicals now, or soon to be, transported in bulk in adjacent cargo holds were to be evaluated experimentally. It has been estimated that over a hundred thousand new organic chemicals are synthesized each year in the U.S. but only a small fraction of these ever become sufficiently useful to be used or shipped in bulk. A low-cost way to estimate potential hazard at the research and development stage (which might entail use or transportation of small, but still highly hazardous, quantities of material) would be valuable.

Simplification and improvement of hazard rating systems could be undertaken using a successful computer simulation of chemical hazard. Many of the current hazard rating systems are quite subjective and may thereby impose unnecessary restrictions (e.g., use, processing or transportation cost penalties) on some chemicals while allowing others to present excessive risks to human life, the environment, transportation facilities, and equipment. The cost and time penalities for such errors in current hazard rating systems could be reduced by an impartial but accurate computer assessment of hazard. Unanticipated hazards, which might slip through an experimental hazard test program due to, for instance, critical sample geometry effects such as frequently encountered in explosive testing (representing the worst hazard), might be identified if a successful computer simulation is possible. In all these potential benefit areas, even partial success of a computer simulation would be useful to serve as a screening tool which could concentrate the comparatively expensive experimental evaluations on those chemicals which pose the greatest hazard.

BACKGROUND

A number of recent studies have attempted to use thermodynamic evaluations to predict chemical hazard, defined by the National Fire Protection Association (NFPA) as "reactivity rating" (Stull 1970, Stull 1974, Davis and Ake 1973) or "experimental shock sensitivity data" (Treweek *et al* 1973). Only recently, however, has anyone attempted to relate calculated parameters with experimental hazard data or with other consensus rating systems or to assess the relative power of the various combinations of calculated thermodynamic parameters and experimental data.

This study (Alexander *et al* 1975, Treweek *et al* 1975/1976) concluded that all the parameters previously proposed could be graded into 3 categories according to their relative power in estimating energy hazard potential:

High	4 CHETAH parameters
	Resonance stabilization of free radical
	P_O
	H_O
Medium	P_D
	T_D
	H_D
	$H_{polymerization}$
Low	T_A
	E_A
	log A

The T, P, and H stand for temperatures, pressures and enthalpies of oxidation (O) or decomposition (D) as predicted by classical thermodynamics (Stull 1970), and E_A and log A are from the Arrhenius rate equation (Stull 1973). Equally important, this study confirmed an earlier observation (Treweek *et al* 1973) that there was no simple relationship between any of these parameters and energy hazard potential. Therefore, the overall

problem is well suited for the more powerful techniques of statistical analysis such as pattern recognition (Kowalski and Bender 1972) or automatic interaction detection (AID) (Sonquist and Morgan 1964) rather than conventional regression analysis.

It is interesting to note that the U.S. National Bureau of Standards considered the same problem on two projects (Tsang and Domalski 1974, Domalski 1977) and, using less rigorous and less sophisticated approaches, came to the conclusion that "the predictive schemes as they now exist do not justify any high degree of confidence." In these National Bureau of Standards studies, however, classical regression analysis, linear discriminate analysis (Dixon 1964), probit analysis (Pearson and Hartley 1958), or even simple rankings (Davis and Ake 1973) were not attempted as recommended by the authors in the ASTM's user manual for CHETAH (Seaton *et al* 1974).

CONSENSUS STABILITY (SELF-REACTIVITY) HAZARD RATING SYSTEMS

Detailed study of current hazard rating systems reveals a marked difference in the definition of terms like "reactivity," a vast difference in the degree of subjectivity required to assign a given chemical to a particular hazard class, and in some cases a lumping of more than one type of hazard into the same rating system to facilitate use by a particular group. All of these systems have a range of hazard ratings from 0 to 4, where 0 is the least hazardous.

To exemplify the diversity of these hazard rating systems, the U.S. National Academy of Sciencies—National Research Council (National Academy of Science 1973) system, developed for the U.S. Coast Guard, breaks reactivity into 5 distinct rating systems: *other chemical*, *binary compatibility*, *water*, *self* (table 1), and *fire*. The National Fire Protection Association (1973) lumps many of the same considerations into 2 systems: *reactivity* (table 2) (shock sensitivity, decomposition or polymerization and reaction with water) and *flammability* (ignition and explosive dusts).

The NFPA Manual of Hazardous Chemical Reactions 491 M (NFPA 1973) is not really a rating system in the same sense, but rather a compendium of binary chemical systems known to react "hazardously." Therefore, it was not considered. Similarly, the U.S. Department of Transportation (DOT 1973) classification of hazardous materials according to the greatest hazard present (except for Class A poisons or radioactive materials when both hazards are classified) is difficult to interpret if information about a hazard less than "the greatest" is desired.

TABLE 1

U.S. Coast Guard (National Academy of Sciences-National Research Council) Self-Reactivity Hazard Rating System.

Grade	
0	No appreciable reaction
1	React under certain conditions but non-hazardous.
2	React if contaminated by initiator—may be hazardous. Do not require stabilizer.
3	May be hazardous—require stabilizer.
4	Hazardous self-oxidations or explosions.

TABLE 2

National Fire Protection Association Reactivity Hazard Rating System.

Grade	
4	Shock sensitive at normal T and P.
3	Shock sensitive but require strong initiating source or high T and P, or react explosively with water.
2	Unstable, capable of violent chemical change but not detonation or react violently with water.
1	Unstable at high T and P or react slightly with water.
0	Stable and unreactive with water.

For the purposes of this study the consolidations, simplifications and equivalences shown in table 3 were made between the NAS–NRC *self* rating system and the NFPA *reactivity* system. Whenever reactivity with water was felt to influence the NFPA rating, the NAS–NRC *water* rating was consulted and appropriate adjustments considered. It is felt that these consolidations are more than justified after consideration of the rela-

TABLE 3
Consolidated Rating System for Self Reactivity of Hazard Rating Systems.

Class Number and Project Characterization	USCG–(NAS–NRC)* Self	NFPA** Reactivity
1 Nonhazardous	0, 1***	0
2 Hazardous decompositions or polymerizations	2, 3	1, 2
3 Explosives	4	3, 4

*NAS–NRC, 1973, (National Academy of Sciences-National Research Council).
**NFPA, 1973, (National Fire Protection Association).
***See Grades Tables 1 and 2.

tive lack of discrimination between NAS–NRC *self* grades 0 and 1 (both nonhazardous reactions) and grades 2 and 3 (reflecting the stabilizer requirement more than the severity of the chemical reaction), and between NFPA *reactivity* grades 1 and 2 (both capable of hazardous reactions but not explosions) and grades 3 and 4 (both capable of explosion at unspecified levels of initiation conditions). It was noted, however, that there was no complete reconciliation between the ratings for some of the chemicals encountered.

A summary of these discrepancies between the consensus ratings and/or ASTM experimental data for some of the chemicals considered is shown in table 4. Noteworthy is the fact that nitrobenzene is classified as a nonhazardous chemical by both the NAS–NRC and NFPA, but is known to pose a moderate explosion hazard (Federoff 1962), and was even used in airplane bombs in World War I. On the other hand, 2-nitropropane has never been known to detonate in the course of intensive experimental testing, but is still categorized as an explosive by NAS–NRC and NFPA.

CORRELATION OF CHETAH PARAMETERS WITH CONSENSUS RATING

Computer Program CHETAH parameters for the 45 chemicals encountered in previous studies (Alexander *et al* 1975, Tsang and Domalski 1974) were used in conjunction with a binary linear separation pattern recognition program (Kowalski and Bender 1972) to predict the consolidated energy hazard class previously discussed. The basic premise of pattern recognition is that the samples can be considered in an abstract mathematical sense as points in an n-dimensional space with coordinates which are sufficient to properly place the samples in unique classes. One must initially examine objects for which the class or property to be determined is known. If the NAS–NRC and NFPA ratings were consistent when consolidated, the chemical was treated as a known, even when other experimental evidence (e.g., as in the case of nitrobenzene) made the concensus rating questionable. If the chemical was not rated by either system it was treated as an unknown, with the exception of unquestionable explosives and detonators. In order to accomodate the pattern recognition program requirement for single-valued functions, CHETAH cri-

TABLE 4
Controversial Chemicals Self-Reactivity.

Chemical	(NAS–NRC, 1973) Self	NFPA (1973) Reactivity	ASTM†	Consolidated Rating*
Hydrazine (anhydrous)	4	2		2 or 3
Nitroethane	4	3	1**	1 or 3
Acetaldehyde	1	2		1 or 2
2-nitropropane	4	3		2 or 3
Nitrobenzene	1	0	3	1 or 3
Toluene-2, 4-diisocyanate	3	1		1 or 2
Acetic acid (glacial)	0	1		(H_2O reactivity) 1 or 2

†American Society for Testing and Materials, Seaton *et al* 1974.
*See Table 3.
**Negative tests with dropped weight and No. 9 detonating cap, 50-gm tetryl tests not run.

terion 3, Oxygen Balance, was treated as two parameters: Parameter No. 3-zero or positive values and Parameter No. 5-negative values.

Analysis results are shown in tables 5 and 6 and the relative weights of variables used in assigning the knowns to their classes are in table 7, along with the optimum vectors developed by a pattern recognition program to decide in which class a given sample belonged. These vectors take the form:

TABLE 5

CHETAH Classification of Chemicals According to Consensus Self-Reactivity Hazard.

CORRECTLY CLASSIFIED CHEMICALS

Chemical	Known Class*	Est. Class
Hydrogen peroxide (50%)	2	2
Ethylene oxide	3	3
Ethylenimine	2	2
Nitroethane	3	3
Vinylidene chloride	2	2
Epichlorophydrin	2	2
2-nitropropane	3	3
Acrylonitrile	2	2
Methyl vinyl ketone	2	2
Styrene	2	2
Aniline	1	1
Butyraldehyde	1	1
Ethylenediamine	1	1
Propylene oxide	2	2
Vinyl acetate	2	2
Acrolein	2	2
Mercury fulminate	3	3
Silver azide	3	3
Lead azide	3	3
Nitroglycerin	3	3
Ethylenedrinitranine	3	3
Ethyl nitrate	3	3
Trinitrotulune	3	3
Azoethane	3	3
Diacetyl peroxide (25%)	3	3
Peracetic acid (60%)	3	3
Vinyl chloride	2	2
Ethylene	2	2
Ethyl acetate	1	1
Ethyl chloride	1	1

*See Table 3 for class numbers.

$$\text{VECTOR} = a_o + \sum_{i=1}^{NVR} a_i VAR_i$$

where NVR = number of variables
a = coefficients published
VAR = variables in order listed.

In order to classify additional unknowns, one need only compute the sign of VECTOR: positive values lie on the lower side of the vector and negative on the higher side of the vector consistent with dot product conventions employed in this pattern recognition program.

The total error of less than 9% experienced with the four CHETAH parameters is all overestimation, consistent with the goals and philosophy underlying the development of CHETAH by ASTM. Further, one of the over-classified chemicals, nitrobenzene, is known to be more hazardous than the consensus ratings indicate.

Previous work (Alexander *et al* 1975, Treweek *et al* 1975/76) noted high estimation power in a parameter called resonance stabilization of the free radical and medium power in enthalpy of polymerization. Therefore, these two parameters were input to the pattern recognition program along with the four CHETAH parameters. Generally, a sample:parameter ratio of 10:1 or more is most desirable in pattern recognition studies in order to minimize the possibility of artifacts producing unreal favorable results, and, although 45 samples to 6 parameters is not entirely satisfactory, it is still within generally practiced guidelines.

The polymerization enthalpies were taken from the literature (Ham 1967) but could have been calculated by CHETAH with comparable accuracy. The resonance stabilization parameter is simply the bond dissociation energy (BDE) for a hydrogen from methane minus the BDE for the appropriate hydrogen of the saturated analog of the polymerizable chemical (see tables 5 and 6). Although somewhat less error was observed than with the CHETAH parameters alone, the principle error was in underestimation of the hazard. All the explosives were correctly classified, and the consensus class of toluene -2, 4-diisocyanate probably reflects its reactivity with water (inherent in the NFPA rating) more than its tendency for hazardous decomposition or polymerization.

CORRELATION OF CHETAH PARAMETERS WITH EXPERIMENTAL SHOCK SENSITIVITY DATA

ASTM Committee E-27 has compiled shock sensitivity data on 236 chemicals

TABLE 6

CHETAH Classification of Chemicals According to Consensus Self-Reactivity Hazard.

MISCLASSIFIED CHEMICALS

Chemical	Known Class†	4 CHETAH Parameters only		4 CHETAH Parameters plus RS and HP††	
		Est. Class	Error*	Est. Class	Error*
Nitrobenzene	1	2	Ov	1	—
Adiponitrile	1	2	Ov	1	—
Ethanolamine	1	2	Ov	1	—
Toluene-2, 4-diisocyanate	2	2	—	1	U
Total errors and % error			3 (<9%)		1 (<3%)

CHEMICALS WITH UNKNOWN OR UNCERTAIN CLASSES

Chemical	Uncertain Class†	4 CHETAH Parameters	4 CHETAH Parameters plus RS and HS††	Uncertainty Reason**
		Est. Class	Est. Class	
Hydrazine	3	3	3	B
Nitromethane	3	3	3	A
Acetaldehyde	1	2	1	B
Propargyl bromide	3	3	3	A
1-nitropropane	3	3	3	A
Acetic acid	1	1	1	B
Ethylene chlorophydrin	1	2	2	A
1-octene	3	1	1	A
Acetamide	1	1	1	A
Dimethyl ether	1	2	1	A
N-octane	1	1	1	A

*Error key: Ov = overestimated; U = underestimated.
**Reason key: A = Not rated by both NAS-NRC and NFPA or not explosive or detonator.
B = Discrepancy between NAS-NRC and NFPA when consolidated.
†See Table 3.
††RS = Resonance Stabilization; HP = Heat of Polymerization.

(Seaton *et al* 1974), obtained at the increasing input levels of dropped-weight, No. 9 blasting cap and 50-gram pellet of tetryl. In this study, a chemical was considered explosive (Class 2) if a positive test was noted at any of the three input levels. On the other hand, a chemical was considered nonexplosive (Class 1) only if it gave a negative test with all three tests. Chemicals with incomplete data (usually No. 9 cap and/or tetryl) were treated as unknowns unless a positive result was obtained with the dropped-weight test or No. 9 cap.

The results of the pattern recognition analysis using the four CHETAH parameters are shown in tables 8 and 9. In this analysis the third CHETAH parameter, oxygen balance, was changed in sign for the 2 positive values encountered, and the fourth parameter, Y, was given values of 1, 2, or 3 corresponding to the low, medium, or high energy hazard designations predicted by the program. Historically, peroxides and azides were automatically categorized as hazardous on the basis of their structure. For this study, however, we chose to ignore this practice and examine the consequences. Although the total error (12%) is reasonable using the four CHETAH parameters, the relatively high underestimation (8%) is unacceptable by the committee's goals. It is noted, however, that nearly all of this underestimation error is due to peroxides. With this in mind, an additional parameter, the number of peroxide bonds in the molecule, was included. Only two atyp-

TABLE 7

*Linear Discriminate Vector Coefficients Used to Classify Chemicals in Tables 5 and 6.**

PATTERN RECOGNITION VECTOR COEFFICIENTS

4 CHETAH Parameters**

Parameter (rel. weight)	a_o	a_1 (0.30)	a_2 (0.34)	a_3 (0.21)	a_4 (0.40)	$a_{neg\ 3}$ (0.42)
Classes						
1 & 2	.160457E+01	.633235E+01	+.594177E+01	−.400042E−01	.415545E−01	.172086E+00
1 & 2	−.705900E+00	.169125E+01	.507648E+00	.117851E+00	.702009E−02	−.263703E−01
2 & 3	−.493125E+00	.128289E+01	.582003E+00	.842427E−01	.346431E−02	−.268230E−01

4 CHETAH Parameters plus RS and HP***

Parameter (rel. weight)	a_o	a_1 (0.30)	a_2 (0.34)	a_3 (0.21)	a_4 (0.40)	$a_{neg\ 3}$ (0.42)	a_{RS} (0.52)	a_{HP} (0.26)
Classes								
1 & 2	.181691E+01	.241411E+01	−.350286E+01	−.781495E−01	.105167E−01	.103046E+00	−.464167E−01	−.551864E−01
1 & 3	−.862503E+00	.154322E+01	.543654E+00	.129958E+00	.624395E−02	.277729E−01	−.206806E−01	−.372586E+00
2 & 3	−.578434E+00	.978845E+00	.449689E+00	.861132E−01	.377098E−02	−.211775E−01	−.602008E−03	.653949E−01

*Vector $= a_o + \sum_{i=1}^{NVR} a_i \, Var_i$

**See page 245.

***RS = Resonance Stabilization, HP = Heat of Polymerization.

TABLE 8

CHETAH Classification of Chemicals According to Experimental Dropped Weight and Shock Impact Data.

Misclassified Chemicals	Known Class	4 CHETAH Parameters		4 CHETAH Parameters and Peroxide Bonds	
		Estimated Class	Error*	Estimated Class	Error*
Tertiary butyl perbenzoate	2	1	U	2	—
Acetyl cyclohexylsulfonyl peroxide	2	1	U	2	—
(structure 34)	2	1	U	2	—
Bis (1-hydroxycyclohexyl) peroxide	2	1	U	2	—
Succinic acid peroxide	2	1	U	2	—
Decanoly peroxide	2	1	U	2	—
Number 17 structure (peroxide)	2	1	U	2	—
Boric acid	2**	1	U	1	**
Oxalic acid dihydrate	2**	1	U	1	**
M-nitrobenzoyl chloride	1	2	Ov	2	Ov
4-acetimido-2-nitroanisole	1	2	Ov	2	Ov
4-chloro-3-nitrobenzene sulfonamide	1	2	Ov	2	Ov
Acetonitrile	1	2	Ov	2	Ov
Total errors and % errors			13 (11.7%)		4 (3.6%)

*Error key: U = underestimated; Ov = overestimated.

**Boric acid and oxalic acid were put in this category because of positive test results, but subsequent evaluation showed endothermic decomposition as opposed to detonation.

ical compounds, boric acid and oxalic acid dihydrate, were underestimated (see table 8).

These two compounds have subsequently been shown to undergo endothermic decompositions but not exothermic detonations, so the CHETAH computer classification is actually correct. The remainder of the 236 chemicals listed (Seaton *et al* 1974) were correctly classified by the vector coefficients in table 8. A subroutine for use with the CHETAH program is available from the principal author to provide accessments automatically using the vector discriminants described in this paper.

The ASTM computer program CHETAH will estimate the explosive hazard of any organic chemical containing three or more carbon atoms with nil underestimation error, and less than 4% overestimation error. When CHETAH's four parameters are coupled with heat of polymerization and a resonance stabilization factor, estimation of hazard potential according to consensus grading into three categories: nonhazardous, hazardous decompositions or polymerizations, and explosives can be achieved with comparable accuracy.

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TABLE 9

*Linear Discriminate Vector Coefficients Used to Classify Chemicals in Table 8.**

PATTERN RECOGNITION VECTOR COEFFICIENTS

4 CHETAH PARAMETERS**

Parameter (relative weight)	a_o	a_1 (0.762)	a_2 (0.630)	a_3 (0.685)	a_4 (1.000)
Classes 1 & 2	.849751E+00	−.210673E+00	.745075E−01	−.245606E−02	−.808848E+00

4 CHETAH Parameters and No. Peroxide Bonds

Parameter (relative weight)	a_o	a_1 (0.762)	a_2 (0.630)	a_3 (0.685)	a_4 (1.000)	a_{PB} (0.291)
Classes 1 & 2	.946280E+00	−.343493E+00	.382966E−01	−.237777E−02	−.913971E+00	−.860315E+00

*Vector $= a_o + \sum_{i=1}^{NVR} a_i \, Var_i$

**See page 245.

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